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1991 J. Phys. A: Math. Gen. 24 L61

(http://iopscience.iop.org/0305-4470/24/2/002)

J. Phys. A: Math. Gen. **24** (1991) L61–L62. Printed in the UK

LETTER TO THE EDITOR

Spin tunnelling: a perturbative approach

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Received 20 November 1990

Abstract. It is shown that the tunnelling splitting of the energy levels of the easy-axis spin system in a small transverse magnetic field can be calculated perturbationally for arbitrary S. The results are exact, in contrast to those obtained previously in the same limit by indirect and rather difficult methods.

A quantum spin with the easy-axis anisotropy in a transverse field h described by the Hamiltonian

$$\mathscr{H} = -DS_z^2 - hS_x \tag{1}$$

is an example of a tunnelling system consideration which may be in some respect more convenient than that of a particle tunnelling in an external potential due to the finiteness of the spectrum of the spin operator and the simplicity of matrix elements. Recently the spin tunnelling problem has drawn the attention of researchers [1-5], who calculated the tunnelling splitting of the ground and excited states degenerate pairwise in the case $h = 0$. Among the theoretical methods applied to the spin tunnelling problem were the instanton technique based on a semiclassical representation of the spin system [2], as well as the WKB method [3] and the instanton technique [5] with a mapping onto a particle problem. These methods applicable in the limit $S \gg 1$ are rather involved, including that of [3] where consideration was restricted to the case $h \ll SD$.

Here I will show that in the small field limit the problem may be solved in an elementary way for arbitrary S with the help of perturbation theory. Indeed, the tunnelling splitting ΔE_m of two degenerate states with spin projections $\pm m$ appears, minimally, in the $2m$th order in $h/(SD)$ (see e.g., [6]):

$$\Delta E_m = 2V_{m,m-1}\frac{1}{E_{m-1}-E_m}V_{m-1,m-2}\frac{1}{E_{m-2}-E_m}\cdots V_{-m+1,-m} \tag{2}$$

where

$$V_{M+1,M} \equiv \langle M+1|hS_x|M\rangle = \frac{h}{2}l_M \tag{3}$$

$l_M = [(S-M)(S+1+M)]^{1/2}$ and $E_M = -DM^2$.

The product (2) may be easily calculated:

$$\Delta E_m = 2D\left(\frac{h}{2D}\right)^{2m}\prod_{k=-m+1}^{m-1}\frac{1}{m^2-k^2}\prod_{k=-m}^{m-1}l_k = \frac{2D}{[(2m-1)!]^2}\frac{(S+m)!}{(S-m)!}\left(\frac{h}{2D}\right)^{2m}. \tag{4}$$

0305-4470/91/020061+02$03.50

One can check that (4) gives correct results for low spin values, which may be obtained by other methods:

$S=1/2 \qquad \Delta E_{1/2}=h$

$S=1 \qquad \Delta E_1=h^2/D$

$S=3/2 \qquad \Delta E_{1/2}=2h \qquad$ and $\qquad \Delta E_{3/2}=3h^3/(8D^2)$

$S=2 \qquad \Delta E_1=3h^2/D \qquad$ and $\qquad \Delta E_2=h^4/(12D^3)$

etc. In the large spin limit ($S \gg 1$) our result (4) for the ground state splitting with the help of the Stirling formula simplifies to

$$\Delta E_S \simeq \frac{4DS^{3/2}}{\pi^{1/2}}\left(\frac{eh}{4SD}\right)^{2S}. \tag{5}$$

For highly excited levels ($S-m$, $m \gg 1$) (4) reduces to

$$\Delta E_m \simeq \frac{2D}{\pi}\frac{me^{2m}}{(2m)^{4m}}\frac{(S+m)^{S+1/2+m}}{(S-m)^{S-1/2+m}}\left(\frac{h}{2D}\right)^{2m}. \tag{6}$$

Now we can compare our results with those obtained by other authors. Namely, the ground state splitting ΔE_S calculated in [2] for $h \leqslant SD$ with the help of the instanton technique coincides in the limit $h \ll SD$ with (5). The result of [3] obtained with the help of a mapping onto a particle problem may be, after some rearrangement, represented in the form (6) with the replacement $S \pm m \Rightarrow S+(1/2) \pm m$. For highly excited levels it coincides with (6), and for the ground state ($m=S$) differs from (5) by a factor $(e/\pi)^{1/2} \approx 0.93$, which is the artefact of the WKB approximation. In the cases $S \sim 1$ or $m \sim 1$ the method used in [3] fails. It is worth noticing that the approximate method of [3] requires extensive calculations whereas, as we have seen, in the same small field limit ($h \ll SD$) the general and exact results may be obtained in an elementary way. In fact, these results are complementary to those of [2] corresponding to the case $h \leqslant SD$, $S \gg 1$.

Similarly, one can calculate the level splitting in the other situation described by the Hamiltonian

$$\hat{\mathcal{H}} = -DS_z^2 + BS_y^2. \tag{7}$$

For S half integer the level splitting is obviously zero, and for S integer in the limit $B \ll D$ the result is

$$\Delta E_m = \frac{8D}{[(m-1)!]^2}\frac{(S+m)!}{(S-m)!}\left(\frac{B}{16D}\right)^m. \tag{8}$$

Again, for $S \gg 1$ the ground state splitting ΔE_s, which simplifies to

$$\Delta E_S = \frac{8DS^{3/2}}{\pi^{1/2}}\left(\frac{B}{4D}\right)^S \tag{9}$$

coincides with the result of [2].

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